1,4-Dioxane

123-91-1 | DTXSID4020533

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 10.2 days

Global applicability domain: Outside

Local applicability domain index: 3.18e-01

Confidence level: 8.78e-01

Nearest Neighbors from the Training Set

Image not found
2,2-Dimethylbutane
Measured: 880
Predicted: 16.2

Image not found
Decane
Measured: 157
Predicted: 8.71

Image not found
Undecane
Measured: 88.3
Predicted: 8.56

Image not found
Nonane
Measured: 157
Predicted: 8.49

Image not found
Dodecane
Measured: 201
Predicted: 10.6